Statistical Methods Supporting Unsteady, Non-Periodic Flows

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Overview

Concepts & Methodologies

- **Concepts**

  1) **The nature of yes/no (pass/fail) information**
  2) **A nonlinear probabilistic prediction for yes/no (pass/fail) information**
  3) **Non-sampling-based nonlinear uncertainty propagation techniques**
  4) **Optimal De-noising in unsteady, non-periodic flows and application to uncertainty propagation**

Methodologies being developed and used on several AFRL and NASA projects

Overview

Relevance

- **Purpose of SWBLI TIM**

  1) **Understanding the physics of complex unsteady flow problems by *statistical analysis of unsteady data from experiments and simulations***

  2) **Understanding the practical application of traditional statistical tools and exploring the use of *advanced statistical methods* in use today to explore their applicability to complex unsteady flow problems and the governing physics that can be extracted from these method**

  3) **Establishing a guideline (albeit with many caveats and methods for various types of analysis) for how CFD unsteady simulation results can be analyzed in a manner that is *consistent with how experimentalists could operate and what practical mathematicians would agree upon***

Methodologies being developed and used on several AFRL and NASA projects

Concept 1:

The nature of yes/no (pass/fail) information

or

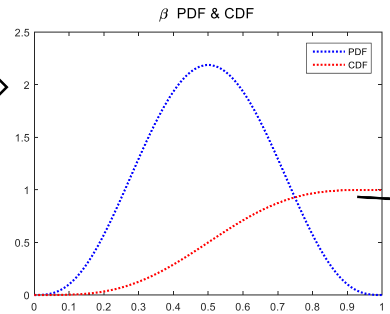
How do we characterize what is likely to cause what we observe?

Concept 1

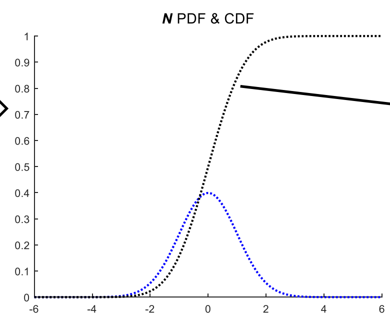
Preliminaries

- **Any ‘humped’ probability density function (PDF) has cumulative distribution function (CDF) that looks like an ‘S’ (sigmoid)**

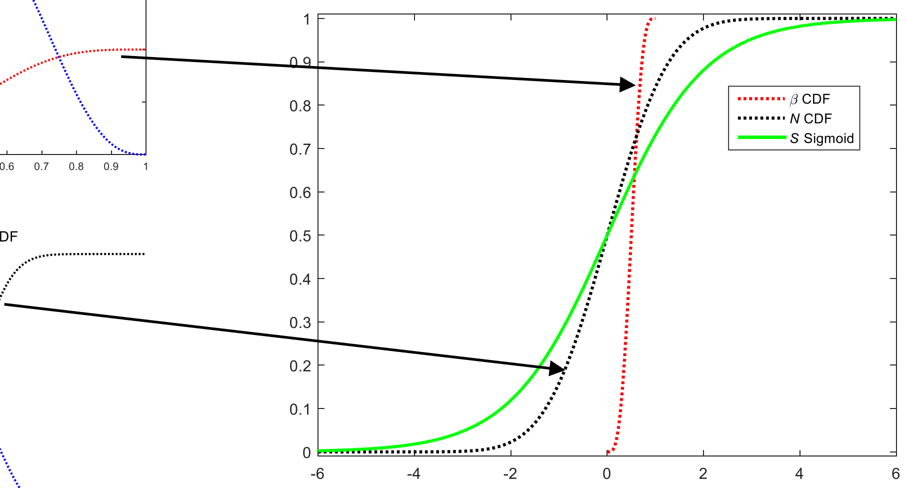
Beta PDF & CDF



Normal PDF & CDF



CDF’s of Beta, Normal, Sigmoid



With stretching & scaling, the sigmoid (‘S’ curve) ~ CDF’s

Concept 1

Theory, 1

- **Sigmoid function for univariate '*x*':**

$$S(x) = \frac{1}{1 + \exp(-x)}$$

- **Sigmoid as special case of logistic distribution:**

$$F_L(x|\mu_L, s_L) = \frac{1}{1 + \exp\left\{-\left(\frac{x - \mu_L}{s_L}\right)\right\}}$$

μ_L **Location parameter**

s_L **Scale parameter**

Given μ_L, s_L, logistic CDF ~ *N*(μ, σ) or beta CDF or …
We now have approximate statistical properties from *N*(μ, σ) → $F_L(x|\mu_L, s_L)$

Concept 1

Theory, 2

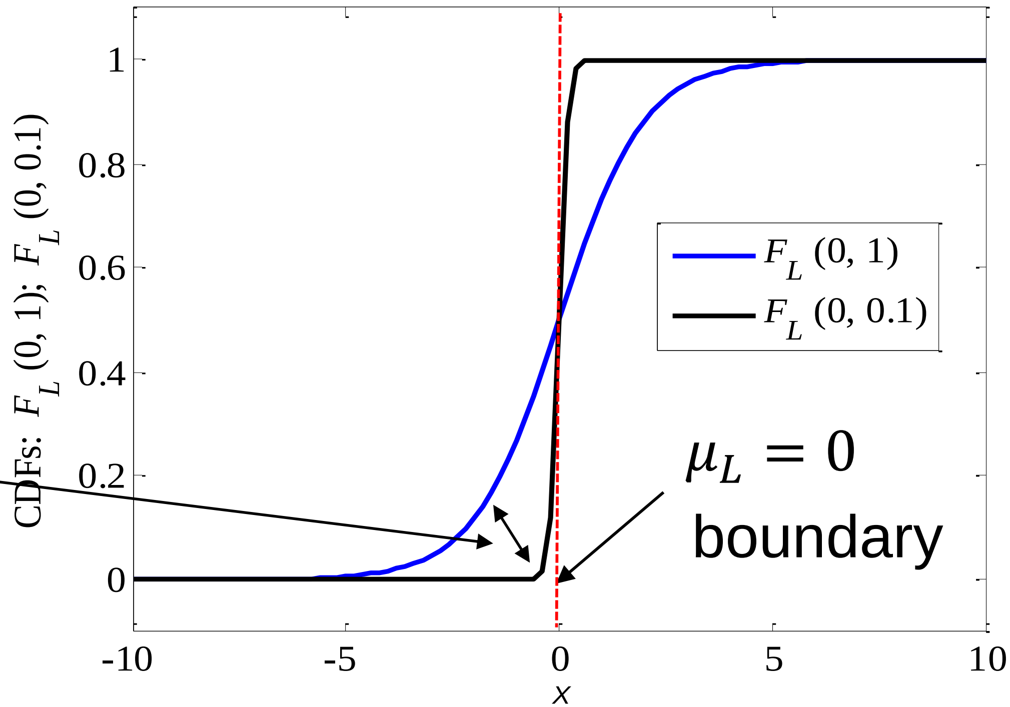
- **Power of logistic distribution → 'shape-change':**

$$F_L(x|\mu_L, s_L) = \frac{1}{1 + \exp\left\{-\left(\frac{x-\mu_L}{s_L}\right)\right\}}:$$

$\mu_L = 0, \text{kept same}$

$s_L = 1 \rightarrow 0.1$

has <u>dramatic</u> influence



Logistic distribution can approximate boundary values from low and high values → e.g. 0 for low, 1 for high & relates to probability space AND pass/fail

Concept 1

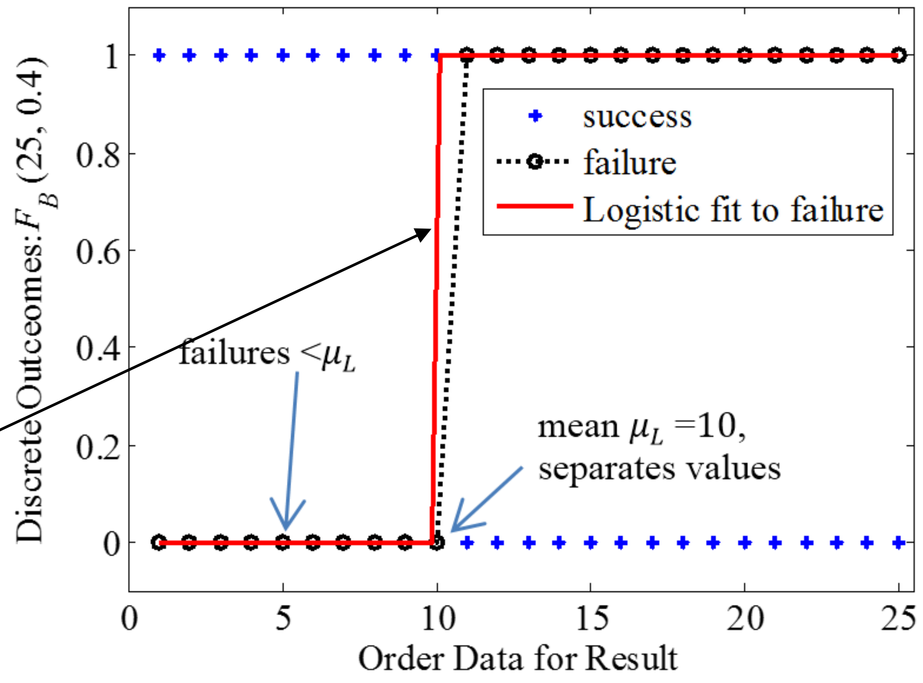
Theory, 3

- **Logistic distribution as discriminator:**

Consider 10 out of 25 failures, then $\mu_L = 10$

Then, 'fit' s_L = 1*10^-3

~ <u>perfectly</u> isolates pass/fails



$$F_L(x|\mu_L, s_L) = \frac{1}{1 + \exp\left\{-\left(\frac{x - \mu_L}{s_L}\right)\right\}}$$

Given $F_L(x|10, 1*10^{-3})$ as 'fit', how to predict?

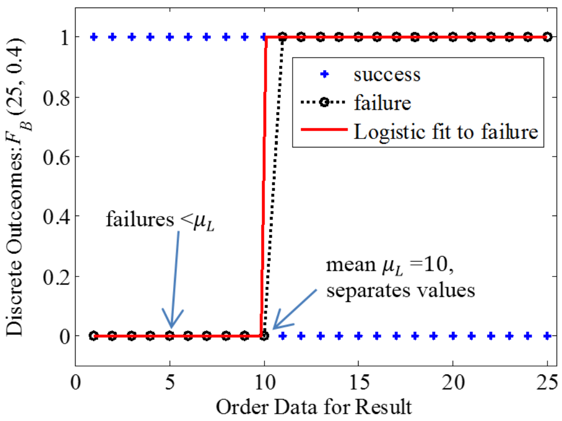
Concept 2:
Develop nonlinear probabilistic prediction for success/failure

Concept 2

Preliminaries

- **Given the logistic distribution as discriminator:**
  - **How to apply this to 'fit' success/failure response and relate to probability theory?**

Given:



Predict probability of success (or failure as complement since only 2 states)

Requires relationship of nonlinear regression to probability theory

Concept 2

Theory, 1

- **Logit function or model relates probabilities**
  - **Provides relationship to odds or probability of success:**

p **is probability event** Y **occurs (success):** $\mathbb{P}(Y = 1)$

ratio of probabilities of success-to-failure is <u>*odds ratio*</u>

$$\text{odds ratio} = \frac{\mathbb{P}(Y = 1)}{\mathbb{P}(Y \neq 1)} = \frac{p}{1 - p}$$

Note:

only 'p' ($\mathbb{P}(Y = 1)$**) needed !**

We can now relate probability theory to fit from data

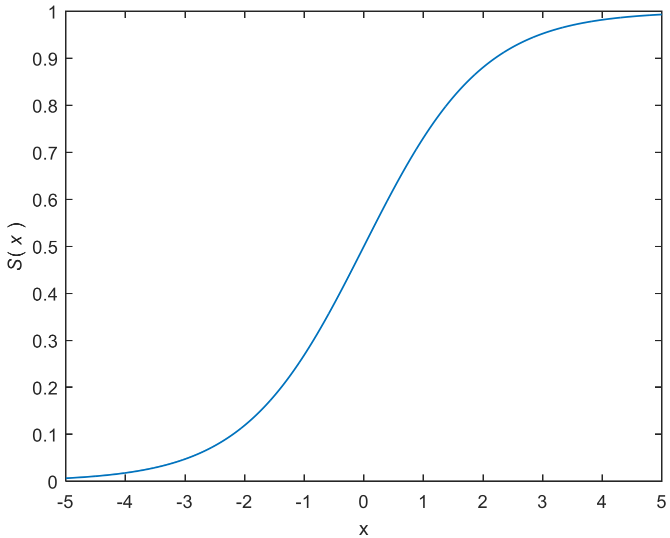
Concept 2

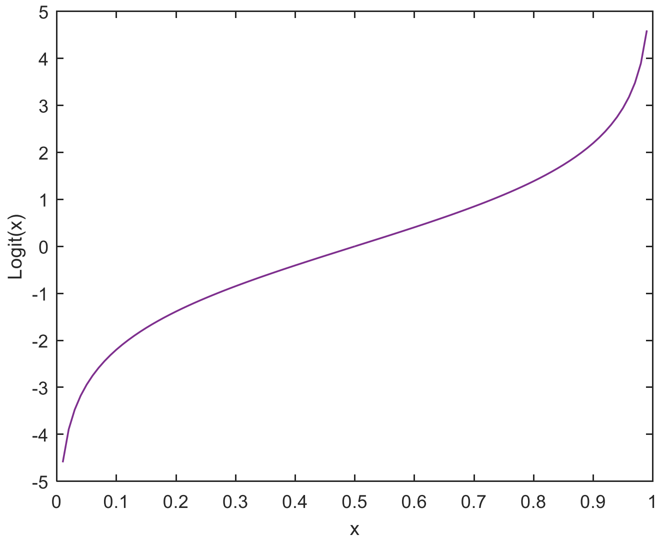
Theory, 2

- **Logit is *inverse* of sigmoid function:**

inverse

$$S(x) = \frac{1}{1 + \exp(-x)} \Longrightarrow Logit(x) = \log\left\{\frac{S(x)^{-1}}{1 - S(x)^{-1}}\right\}$$





$$\text{logit}(p) = \log(\text{odds ratio}) = \log\left\{\frac{p}{1-p}\right\}$$

If parameter is probability ($x = p$), logit is log-odds of success

Concept 2

Theory, 3

- **By extension, logit for multivariate:**

$$L(x) = \left(1 + \exp\left\{-\left[\beta_0 + \sum_{i=1}^{N\ terms} \beta_i x_i\right]\right\}\right)^{-1}$$

β_0 **model constant**

β_i **variable x_i coefficient**

inverse

$$\text{logit}\{L(x)\} = \log(\text{odds ratio}) = \left[\beta_0 + \sum_{i=1}^{N\ terms} \beta_i x_i\right]$$

$L(x)$ **now interpreted as probability that response equals a given value for some linear combination of regressors (Inputs)**

Concept 2

Application, 1

- **Application to realistic scenario:**

$$\text{logit}\{L(x)\} = \log(\text{odds ratio}) = \left[\beta_0 + \sum_{i=1}^{N\ terms} \beta_i x_i\right]$$

Suppose 3 inputs, of different types, and 1 response where

$\boldsymbol{x_1}$**, or A → continuous (e.g. velocity or flow rate)**

$\boldsymbol{x_2}$**, or B → discrete with many states (e.g. angle of attack)**

$\boldsymbol{x_3}$**, or C → binary (e.g. type of aircraft inlet, coded as 0 or 1)**

$\boldsymbol{y}$**, or response → binary (failure coded as 0 or success coded as 1)**

What values of regressor coefficients 'best' describe the probability of success or failure? (e.g. boundary layer transition)

Concept 2

Application, 2

- **Data:**

A → continuous
B → discrete
C → binary
Response → binary (0 or 1)

Data Point #	*Values*			*Response*
	A	*B*	*C*	
1	2.63	20	0	0
2	2.66	20	0	0
3	2.76	17	0	0
4	2.74	19	0	0
5	2.92	12	0	0
6	2.86	17	0	0
7	2.83	19	0	0
8	2.75	25	0	0
9	2.87	21	0	0
10	2.06	22	1	0
11	2.89	22	0	0
12	3.03	25	0	0
13	2.39	19	1	1
14	3.28	24	0	0
15	3.26	25	0	1
16	3.32	23	0	0
17	2.89	14	1	0
18	2.67	24	1	0
19	3.57	23	0	0
20	3.53	26	0	0
21	2.83	27	1	1
22	3.10	21	1	0
23	3.12	23	1	0
24	4.00	21	0	1
25	3.16	25	1	1
26	3.92	29	0	1
27	3.39	17	1	1
28	3.54	24	1	1
29	3.51	26	1	0
30	3.65	21	1	1
31	3.62	28	1	1
32	4.00	23	1	1

Note: I created this data for demonstration purposes only…

Concept 2

Application, 3

- **25 Models considered**
  - **Model 1:**

$$L(x)_1 = (1 + \exp\{-[\beta_0 + \beta_A A]\})^{-1}$$

$$L(x)_{25} = (1 + \exp\{-[\beta_0 + \beta_A A + \beta_B B + \beta_C C + \beta_{AB} AB + \beta_{AB} AC + \beta_{AB} BC$$

Model #	*A*	*B*	*C*	*AB*	*AC*	*BC*	*ABC*
1	1	0	0	0	0	0	0
2	0	1	0	0	0	0	0
3	0	0	1	0	0	0	0
4	1	1	0	0	0	0	0
5	1	0	1	0	0	0	0
6	0	1	1	0	0	0	0
7	1	1	0	1	0	0	0
8	1	0	1	0	1	0	0
9	0	1	1	0	0	1	0
10	1	1	1	0	0	0	0
11	1	1	1	1	0	0	0
12	1	1	1	0	1	0	0
13	1	1	1	0	0	1	0
14	1	1	1	0	0	0	1
15	1	1	1	1	1	0	0
16	1	1	1	1	0	1	0
17	1	1	1	1	0	0	1
18	1	1	1	0	1	1	0
19	1	1	1	0	1	0	1
20	1	1	1	0	0	1	1
21	1	1	1	1	1	1	0
22	1	1	1	1	1	0	1
23	1	1	1	1	0	1	1
24	1	1	1	0	1	1	1
25	1	1	1	1	1	1	1

Models consider independent effects as well as 2- and 3-factor interactions

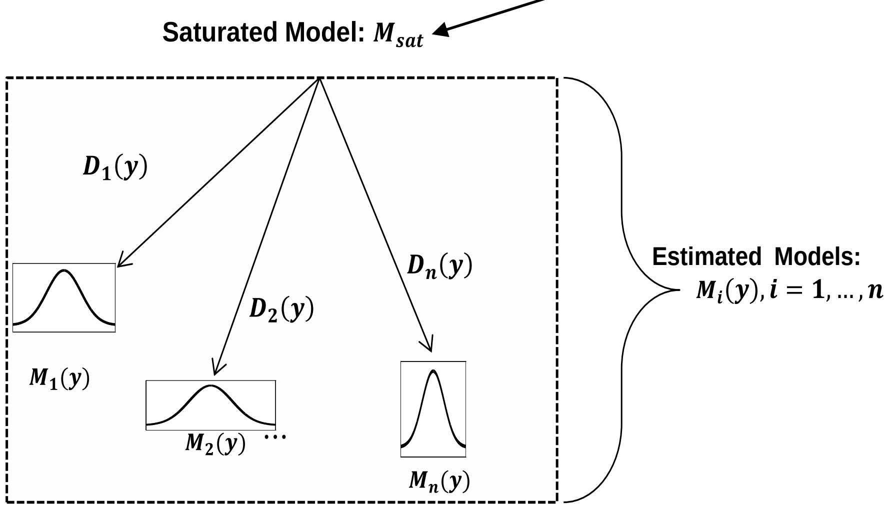
Concept 2

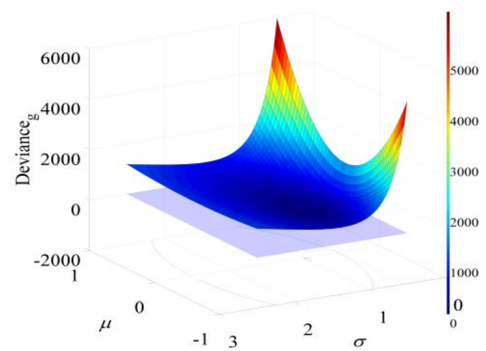
Application, 4

- **Quality metric 1**
  - **Deviance: related to the log likelihood**

$$D(y) = -2\{\log(\mathcal{L}(y|\hat{\theta}_1) - \log(\mathcal{L}(y|\hat{\theta}_{sat}))\}$$

$\hat{\theta}_1$ **model 1 estimated parameters**
$\hat{\theta}_{\mathbf{sat}}$ **full model estimated parameters**
$\mathcal{L}$ **likelihood operator**



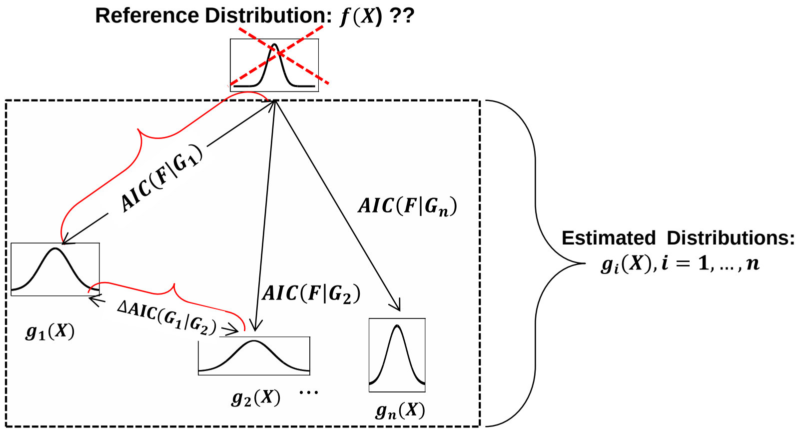


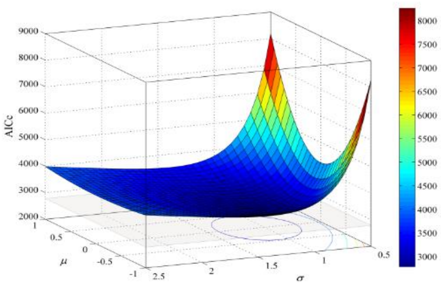
Larger deviance → 'less-well' that the proposed model 'fits' the data

- **Quality metric 2**
  - **Akaike Information Criterion (AIC) related to deviance and therefore to log likelihood**

$$\mathrm{AIC} \equiv -2\mathbb{E}[\,\mathcal{L}(g)] + 2K$$

g **proposed model of data**
K **number of model parameters**
$\mathbb{E}$ **expectation operator**



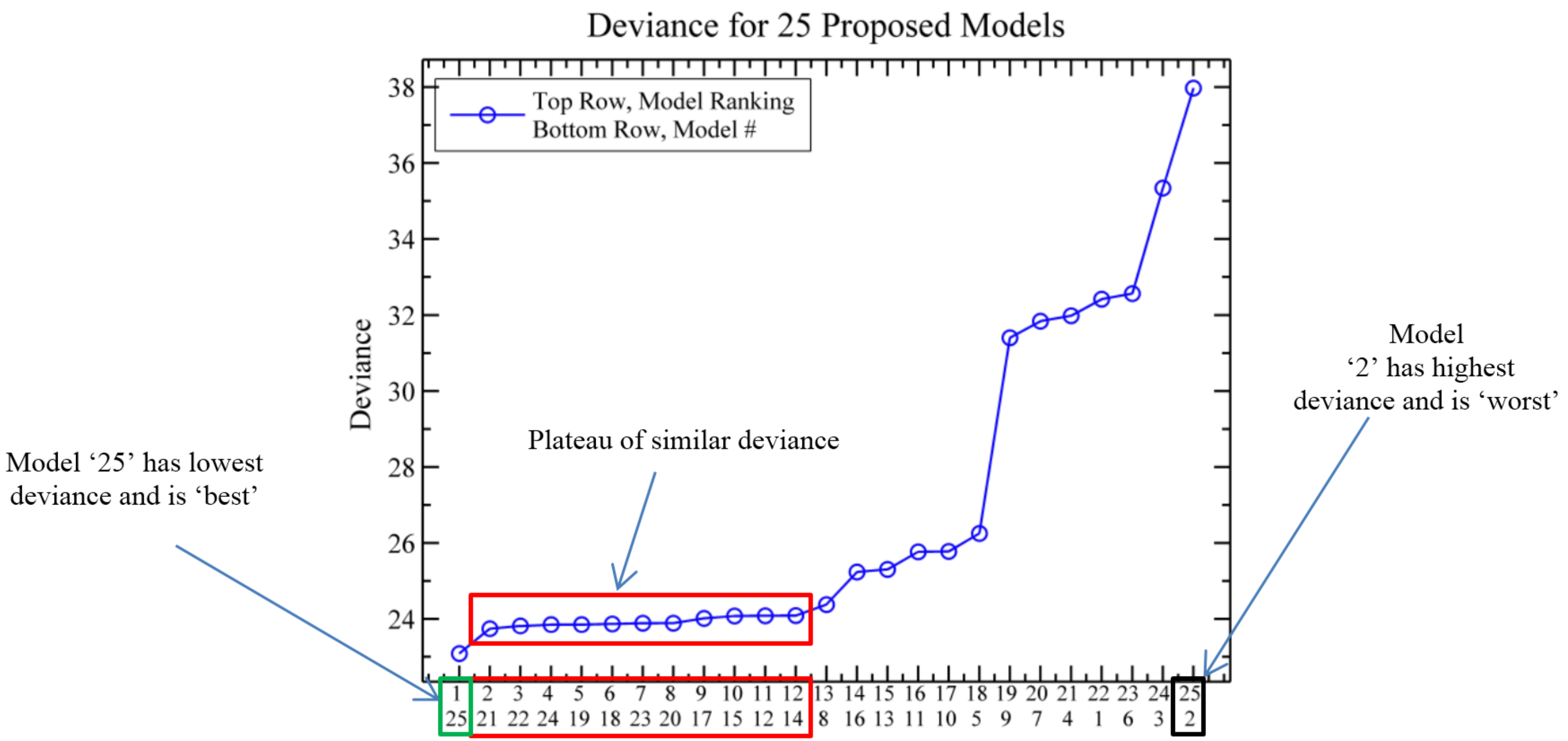


Larger AIC→ 'less-well' that the proposed model 'fits' the data

Concept 2

Results, 1

- **Deviance-based results (typical of stats)**

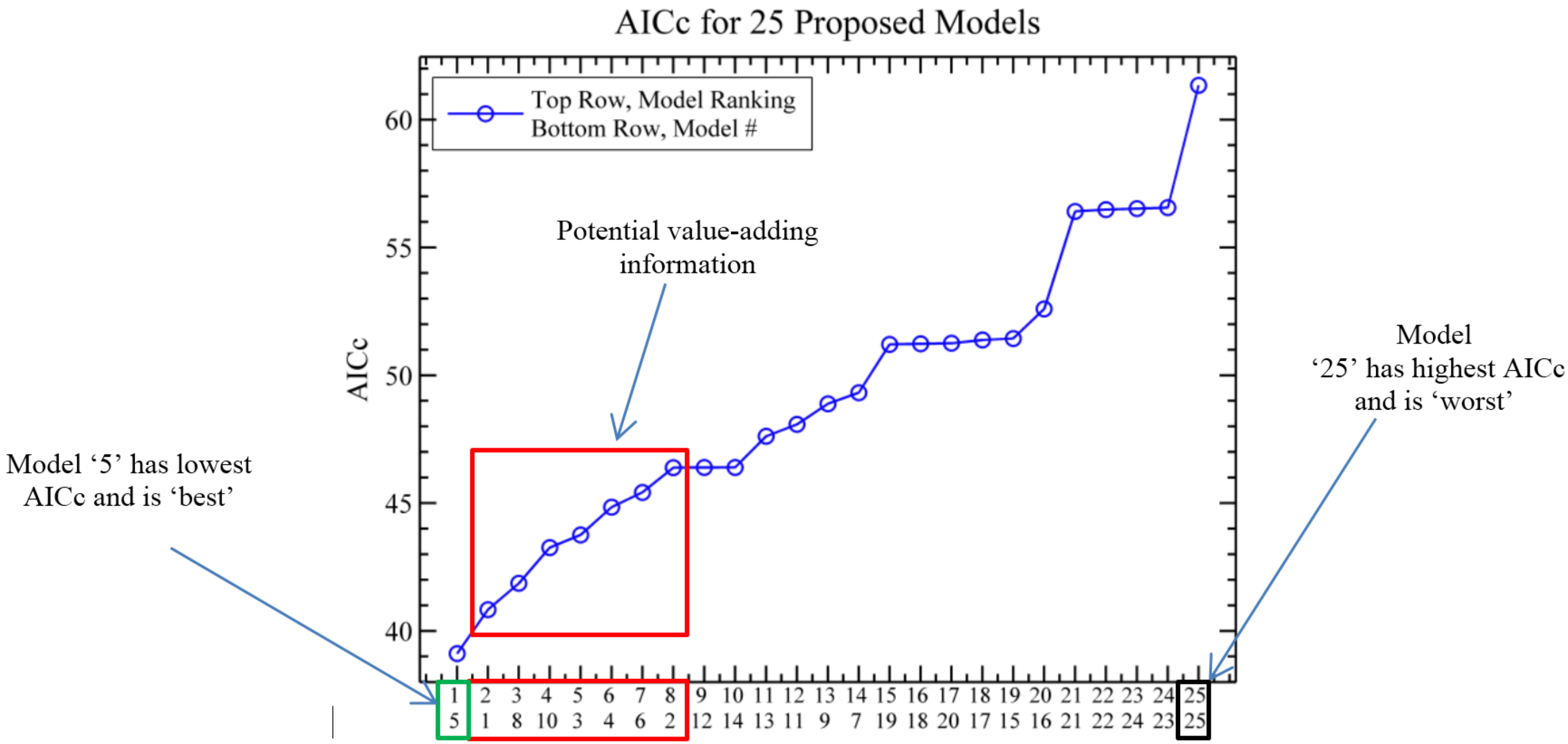


Deviance is prone to 'over-fitting' a la R^2 statistic (more terms are better?)

Concept 2

Results, 2

- **AIC-based results**



AIC avoids 'over-fitting' a la *R*^{2}-adjusted statistic (more terms are *<u>NOT</u>* better?)

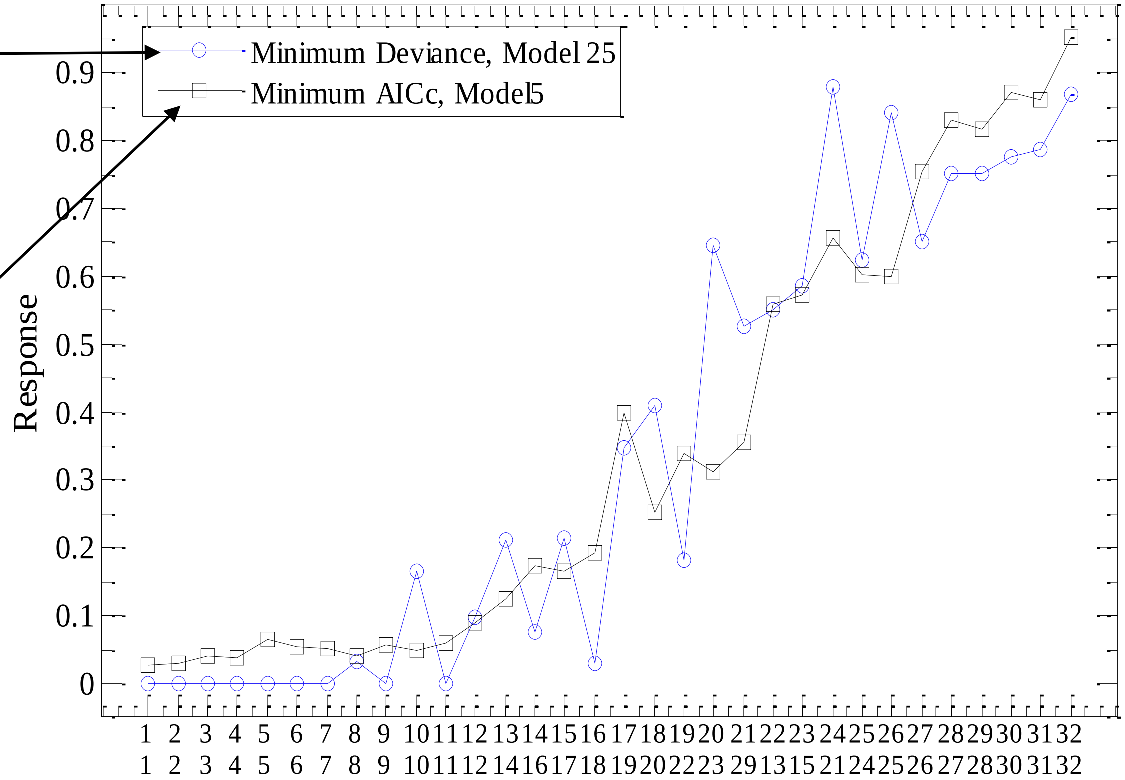
Concept 2

Results, 3

- **Prediction of probabilities**

$L(x)_{25}$
$= (1$
$+ \exp\{-[\beta_0 + \beta_A A + \beta_B B + \beta_C C$
$+ \beta_{AB} AB + \beta_{AB} AC + \beta_{AB} BC$

$L(x)_5$
$= (1$
$+ \exp\{-[\beta_0 + \beta_A A + \beta_C C]\})^{-1}$



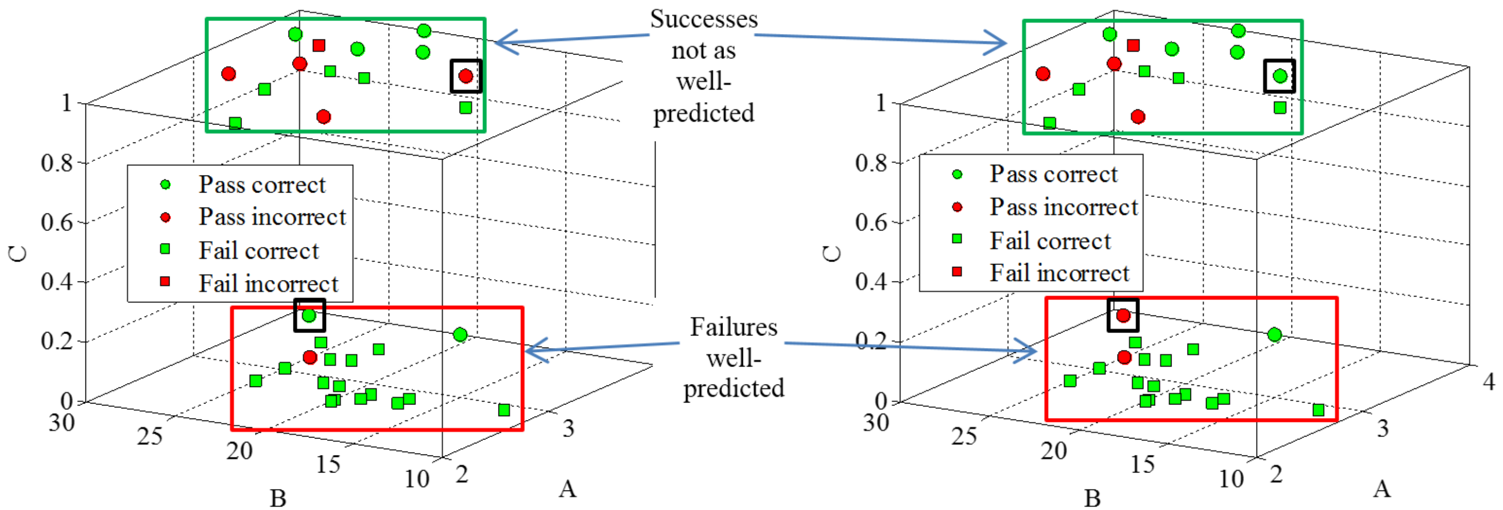
AIC → ~ simplest model while deviance most complex model, but which is better at prediction?

Concept 2

Results, 4

- **Prediction of probabilities (cont'd)**

Deviance **AIC**



			Deviance		AICc	
			Correct	*Incorrect*	*Correct*	*Incorrect*
Actual Result	Fail	0.6563	0.625	0.0313	0.625	0.0313
	Pass	0.3438	0.1875	0.1563	0.1875	0.1563

~Simplest model via AIC *SAME* predictive power as deviance model…

Concept 3:
Non-sampling-based nonlinear uncertainty propagation techniques

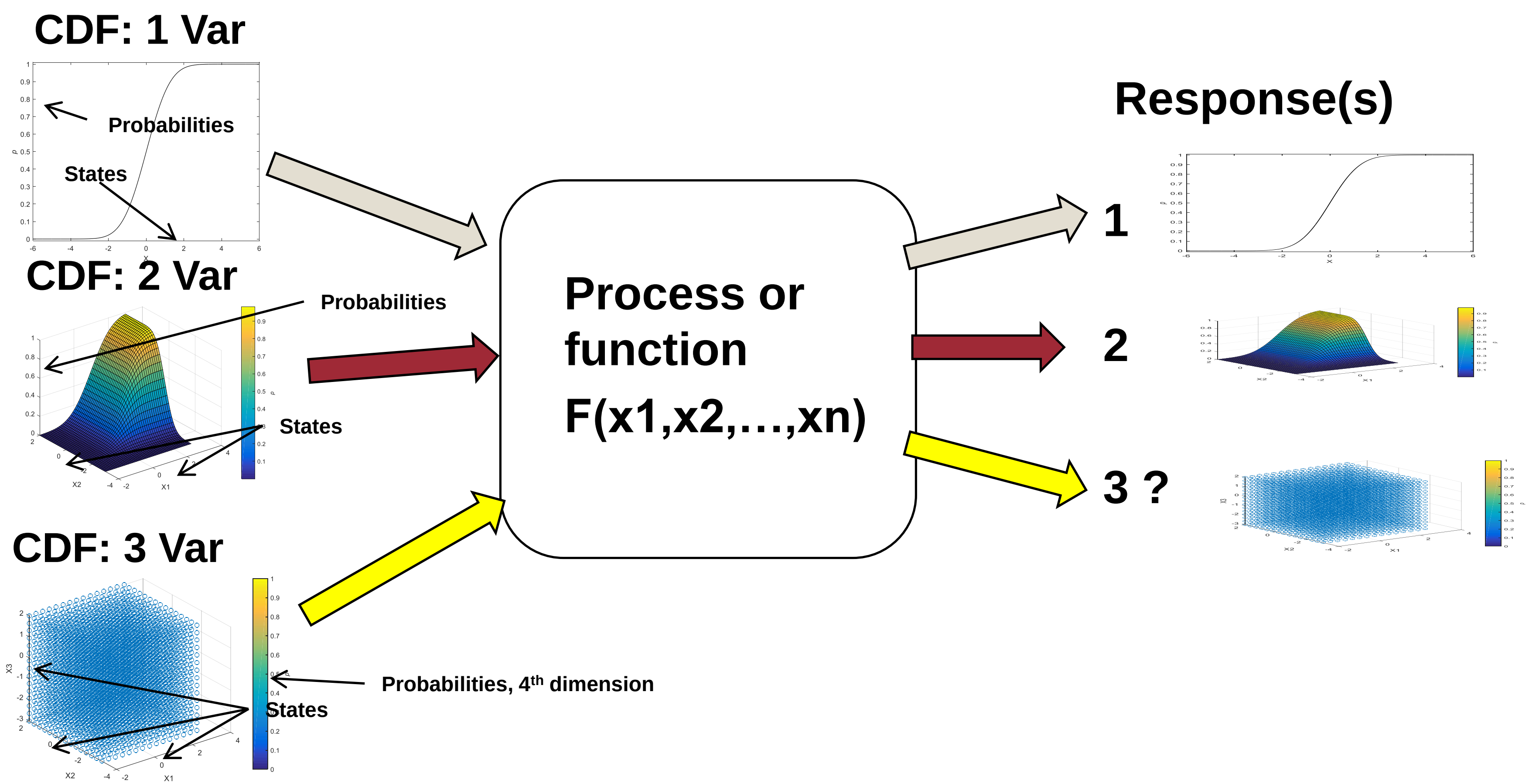
or

Monte Carlo: a method of the past?

Concept 3

Thoughts

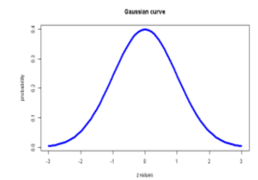
- **Nonlinear uncertainty propagation**



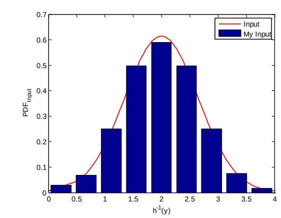
Have 'n' inputs, 'm' outputs completed

Concept 3

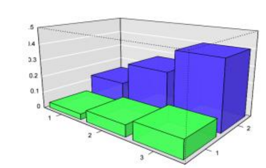
Continuous & Discrete Probability Functions



- **Continuous Probability *Density* Function (PDF):**
  - **Infinite # of points, described as *function*, may be differentiable and integrable → exact solutions in *some* cases (e.g. Normal or Gaussian PDF)**
  - **NOT defined at a point, but in interval**



- **Discrete Probability *Mass* Function (PMF):**
  - **Finite # of points, described as *states*, is summable and differenceable → approximate solutions *all* cases**



Notable differences in concepts *and* implementation, PMF more representative of discrete data acquisition systems (i.e. experimental data)

Concept 3

Nonlinear Uncertainty Propagation

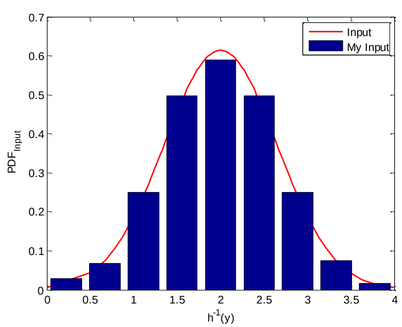
- **Methods investigated / developed**
  - **Theoretical for verification**
  - **Numerical of Theoretical for verification**
  - **Linear approximation of Numerical for verification**
  - **Quadratic approximation of Numerical for verification**
  - **Monte Carlo (1e6 samples)**
  - **New method (don’t have a name for it yet!)**

Extensible to all systems / experiments

Concept 3

New Uncertainty Propagation Method ?

- **Convert input continuous PDF to discrete probability mass function (PMF), then to CDF**
- **Determine weighted sampling schema at discrete points of CDF**
- **Pro-rata weight data reduction equation (DRE)**
- **Determine output PDF via DRE transformation**



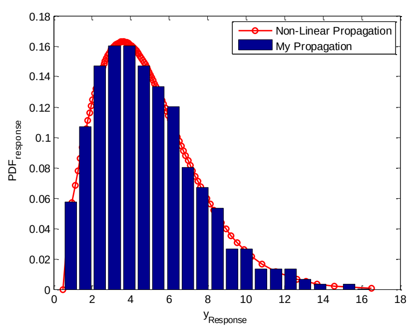
Discrete *Input* PDF → PMF

Data Reduction Equation (DRE)

$Y = f(x)$

Or

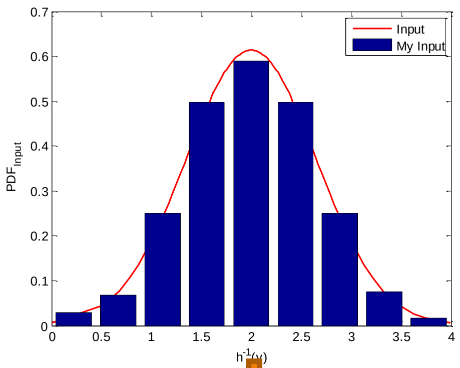
Experiment

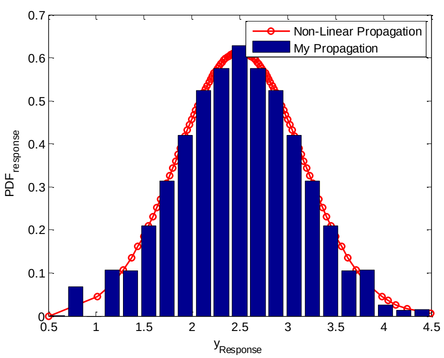


Discrete *Output* PDF or PMF

Concept 3

New UP? Linear Verification Results





Linear | y=x + 1/2

Theory

	means	vars	stds
Finite	2.494771268	0.425539643	0.652333996
Infinite	2.5	0.4225	0.65
Finite (abs)	2.494771268	0.425539643	0.652333996
Infinite (abs)	2.5	0.4225	0.65

Numerical

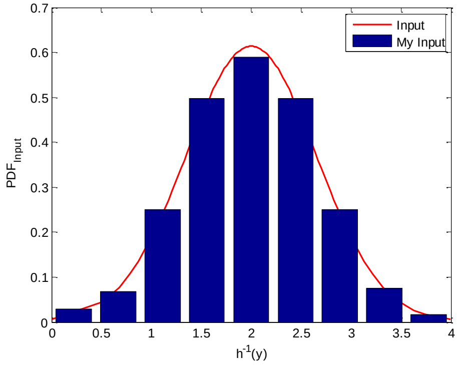
	means	vars	stds
exact	2.500641609	0.41029264	0.640540896
lin_JHD	2.500641609	0.41029264	0.640540896
poly2	1.114163829	0.962013608	0.980822924
MC_infinite	2.500494487	0.422829967	0.650253771
MC_finite	2.497356214	0.421063125	0.64889377
JHD	2.494847852	0.426014749	0.652698054

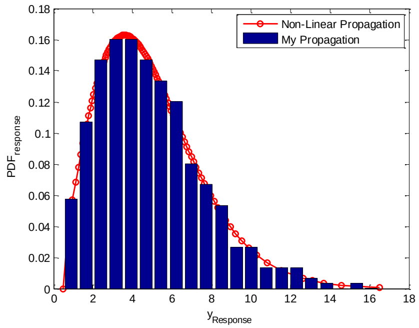
Errors wrt Finite (abs)

	means	vars	stds
exact	0.235305753	-3.58298066	-1.80783161
lin_JHD	0.235305753	-3.58298066	-1.80783161
poly2	-55.3400409	126.0690923	50.35594178
MC_infinite	0.229408555	-0.63676223	-0.31888957
MC_finite	0.10361453	-1.05196255	-0.52737188
JHD	0.003069747	0.111647934	0.055808394

Concept 3

New UP? Quadratic Results





Quadratic

y=x^2 + 1/2

Theory

	means	vars	stds
Finite	4.903083436	6.966151768	2.639346845
Infinite	4.9225	7.1170125	2.667772948
Finite (abs)	4.903083436	6.966151768	2.639346845
Infinite (abs)	4.921325818	7.127881259	2.669809218

Numerical

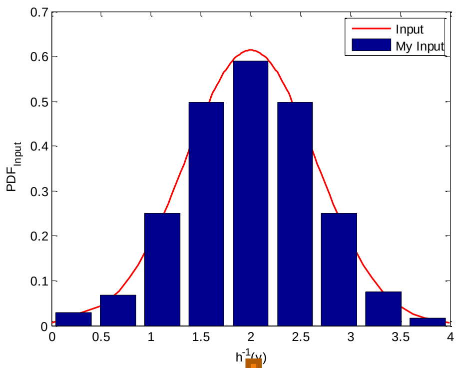
	means	vars	stds
exact	4.908541345	6.840044764	2.615347924
lin_JHD	4.908541345	6.840044764	2.615347924
poly2	4.908376988	6.838715311	2.615093748
MC_infinite	4.919901324	7.108866314	2.666245734
MC_finite	4.905606302	7.056601854	2.65642652
JHD	4.905423798	7.034423318	2.652248729

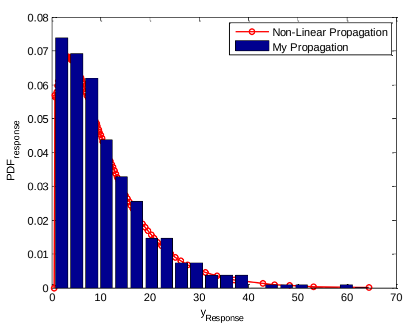
Errors wrt Finite (abs)

	means	vars	stds
exact	0.111315842	-1.81028217	-0.90927499
lin_JHD	0.111315842	-1.81028217	-0.90927499
poly2	0.107963731	-1.82936664	-0.91890525
MC_infinite	0.343006343	2.04868557	1.019149457
MC_finite	0.051454663	1.298422568	0.647117479
JHD	0.047732445	0.980046841	0.488828653

Concept 3

New UP? Cubic Results





Cubic

y=x^3 + 1/2

Theory

	means	vars	stds
Finite	10.95719323	83.57526577	9.141950874
Infinite	11.035	87.67618336	9.363556128
Finite (abs)	10.95719323	83.57526577	9.141950874
Infinite (abs)	11.035	87.67618336	9.363556128

Numerical

	means	vars	stds
exact	10.98184651	82.84892736	9.102138615
lin_JHD	10.98012649	82.71948612	9.09502535
poly2	10.97487045	82.48700319	9.082235583
MC_infinite	11.03568675	87.73723701	9.366815735
MC_finite	10.98354139	86.79472096	9.316368443
JHD	10.97556001	84.77614372	9.207396142

Errors wrt Finite (abs)

	means	vars	stds
exact	0.224996316	-0.86908298	-0.43548975
lin_JHD	0.209298687	-1.02396282	-0.51329879
poly2	0.161329803	-1.30213475	-0.65320073
MC_infinite	0.716365193	4.979907874	2.459703237
MC_finite	0.240464518	3.852162667	1.907881279
JHD	0.167622993	1.436881993	0.715878586

New (?) method for Nonlinear Uncertainty Propagation is *very* fast and introduces minimal uncertainty relative to theory

(21 pts on input PDF w/1e6 samples < 0.1 sec

Concept 4:

Optimal De-noising in unsteady, non-periodic flows and application to uncertainty propagation

or

How much noise, of what type, and how to use it ??

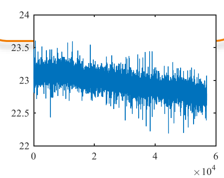
Concept 4

Process For Experimental Uncertainty

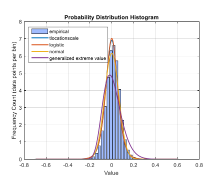
Design the Experiment

Acquire Data

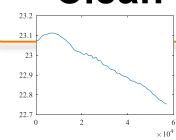
Noisy Raw Data



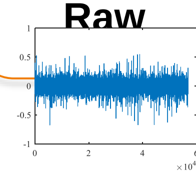
De-Noise then Noise Character and Parameters



De-Noised 'Clean'



Noise of Raw



Uses:

1) Residual mapping,
2) Validation process,
3) 'Cleaner' input to controllers
4) Model comparison,

Uses:

1) Uncertainty characterization,
2) Uncertainty quantification,
3) Uncertainty propagation
4) Unifying filter for sensor <u>output</u>

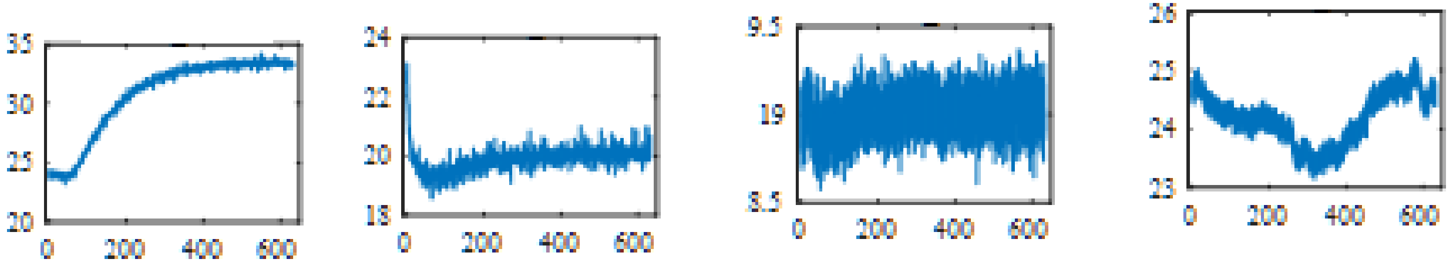
Concept 4

Process For Experimental Uncertainty

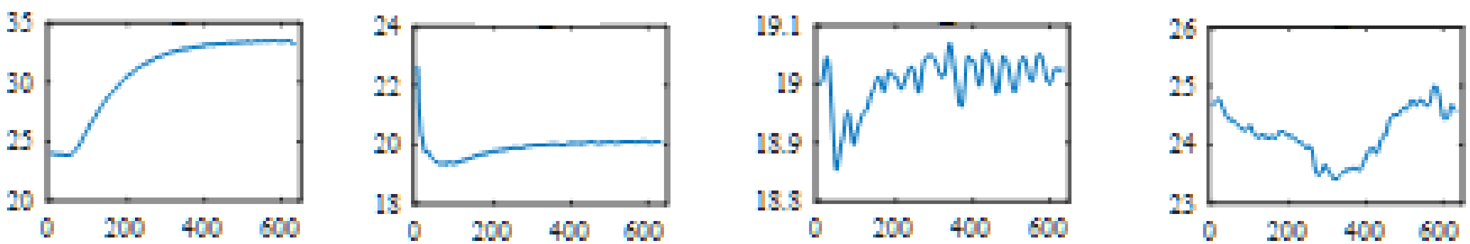
- **Varying patterns of raw signal(t) & denoised(t)**

	1st Order step response w/delay	2nd Order step response w/o delay	~ Stationary response	~ 'Walking' response

Raw



De-noised



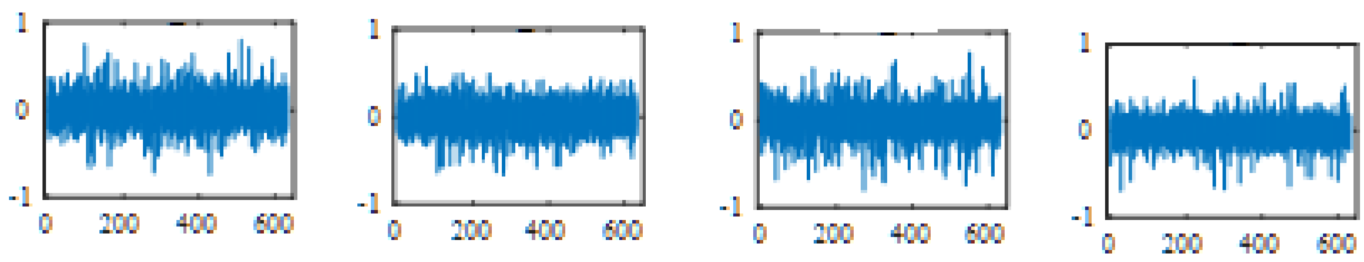
Raw signals difficult to work with due to varying patterns and noise

Concept 4

Process For Experimental Uncertainty

- **Varying patterns of raw signal(t) & denoised(t)**

	1st Order step response w/delay	2nd Order step response w/o delay	~ Stationary response	~ 'Walking' response
Noise				

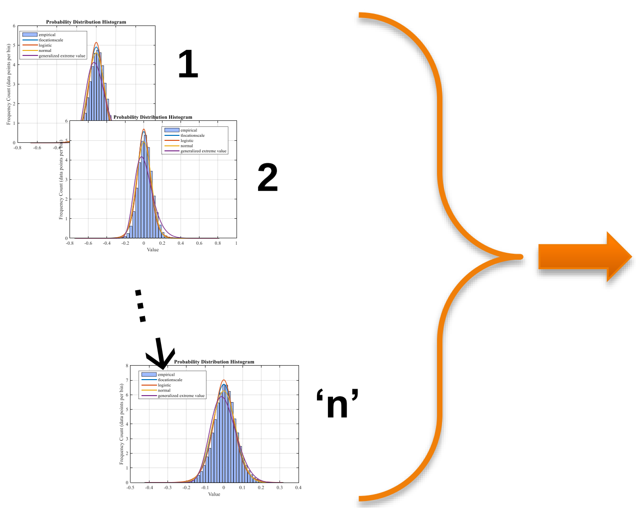


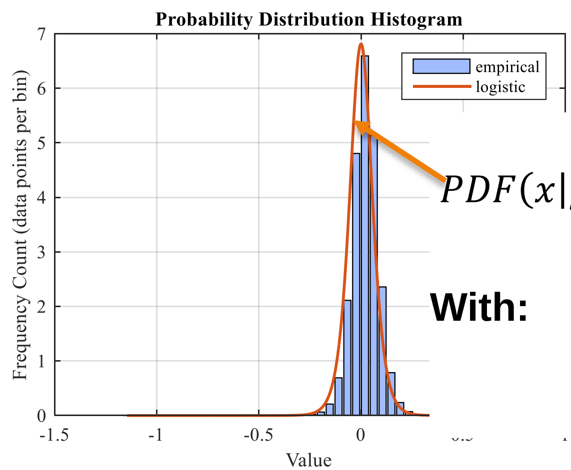
Denoised illustrate same *character* of noise

Concept 4

Process For Experimental Uncertainty

- **<u>Quantitative</u> analysis shows noise ~same**
  - **Same magnitudes and support for logistic function**





$$PDF(x|\mu, scale) = \frac{\exp\left[\frac{x-\mu}{scale}\right]}{scale\left\{1+\exp\left[\frac{x-\mu}{scale}\right]\right\}^2}$$

With:

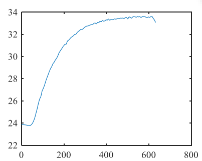
$$(\mu, scale) = (0, 0.037)$$

Concept 4

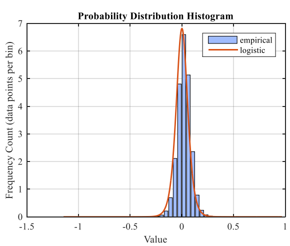
Process For Experimental Uncertainty

- **Given a simulated response for ~same conditions as experiment:**
  - **Use noise PDF to propagate uncertainty via simulation**

Input 'Cleaned'

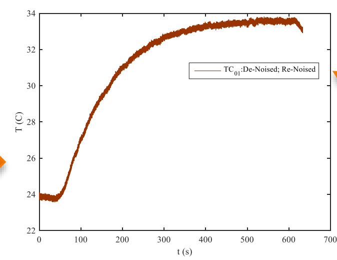


General **noise PDF**



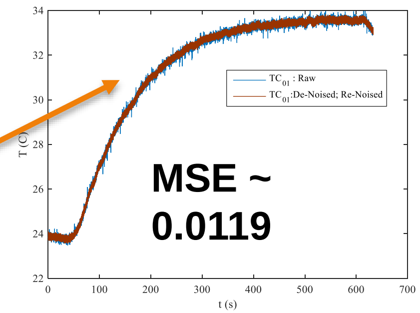
Propagate noise PDF to 'clean' signal

Generated **noisy signal**



Compare *generated* noisy signal to *actual* noisy signal

Actual **noisy signal**



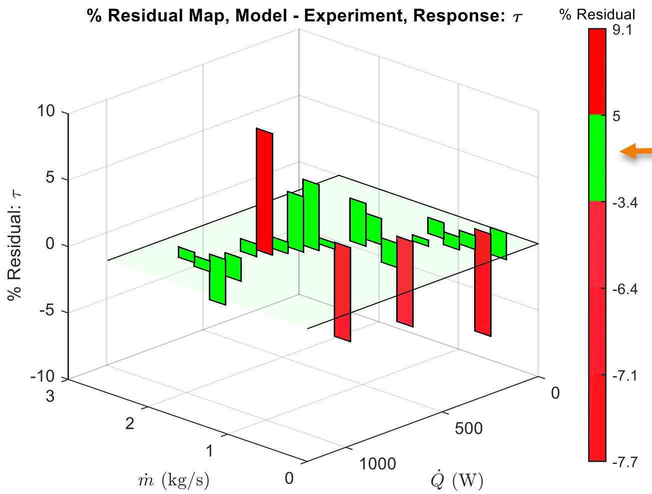
MSE ~ 0.0119

Meaning: We can now use experimentally-determined noise in simulations to realistically capture the operational characteristics of the *true* system's noise

Concept 4

Process For Experimental Uncertainty

- **Create residual map of simulation-to-experiment**



Define 'acceptable' comparison

Plot %residuals as over- or-under-estimated by simulation

Enables visualization of regions of similarities (green) and regions of discrepancies (red)

Meaning: We can now focus on regions where simulations and experiments differ.
Additional concept: use residual mapping to conjoin multi-fidelity CFD simulations ?

Summary

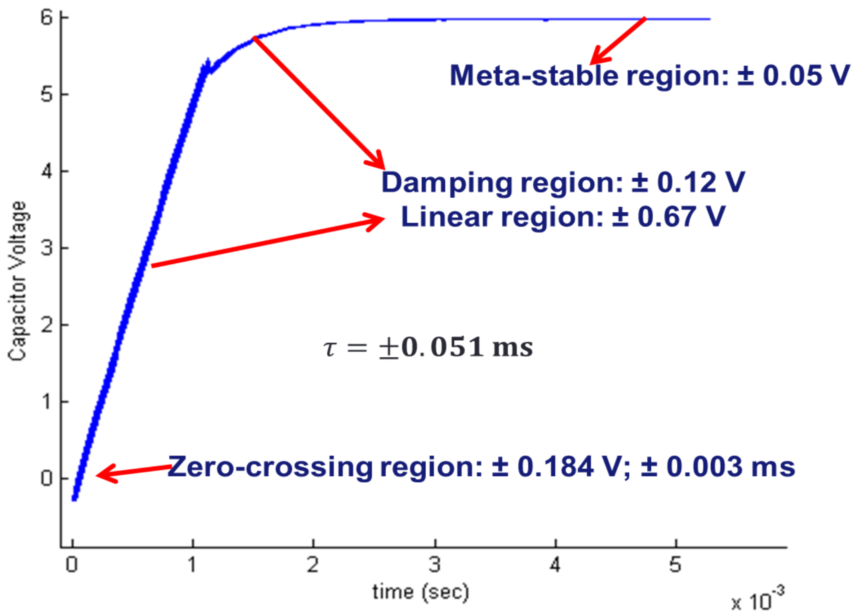
Concepts & Methodologies

- **Concepts**
  1) **The nature of yes/no (pass/fail) information**
     1) **Characterize transition likelihood**
  2) **A nonlinear probabilistic prediction for yes/no (pass/fail) information**
     1) **When/ where/ and under what conditions is transition likely to happen ?**
  3) **Non-sampling-based nonlinear uncertainty propagation techniques**
     1) **Fast, accurate UP for dynamic flows**
  4) **Optimal De-noising in unsteady, non-periodic flows and application to uncertainty propagation**

Bonus: Methodologies *should* be extensible to multiple dimensions for unsteady, non-periodic flows

Quick aside

- **Actual 2nd order undamped experimental signal with noise: note noise character w/time**



Imagine

An ~in-situ UP process based upon ~actual conditions

- **Potential application for 3D experimental**
  1) **Acquire raw data, denoise, characterize, estimate response, propagate uncertainty to response**
  2) **Capture uncertainty in the 3D volume (t)**
     1) **Potentially large 'bursts' of uncertainty in time**
     2) **Is this 'burst' like activation energy in chemical reactions? If so, can help to explain the turbulent transition**

Bonus: Methodologies *<u>should</u>* be extensible to multiple dimensions for unsteady, non-periodic flows